Absorption of IR Radiation in Pool Fires

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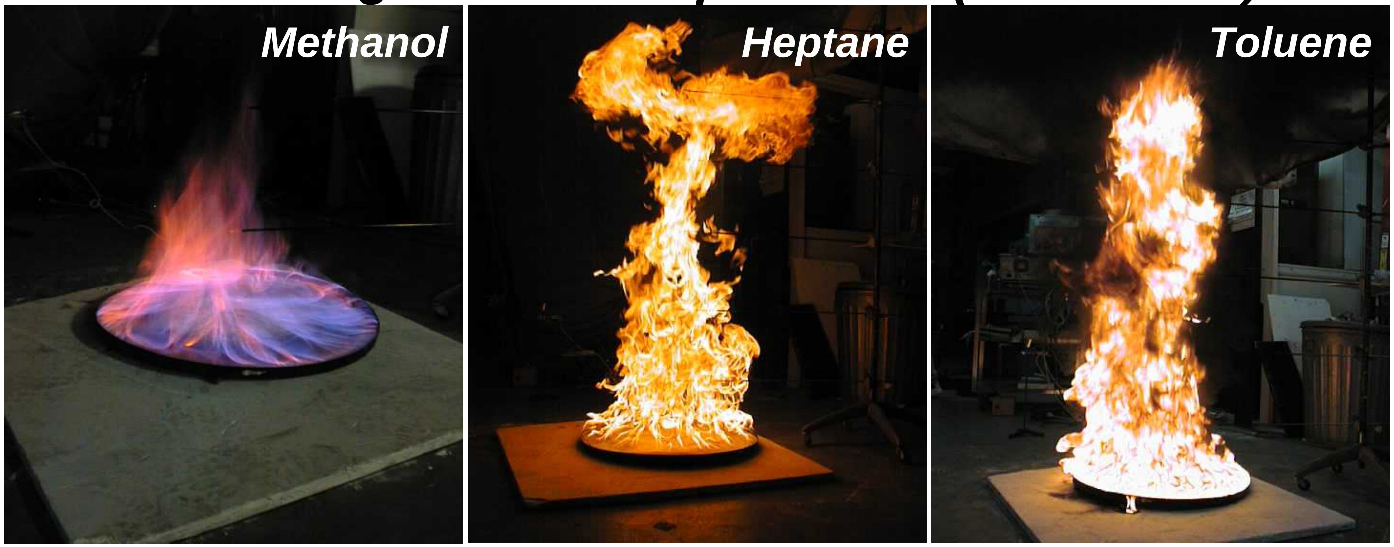
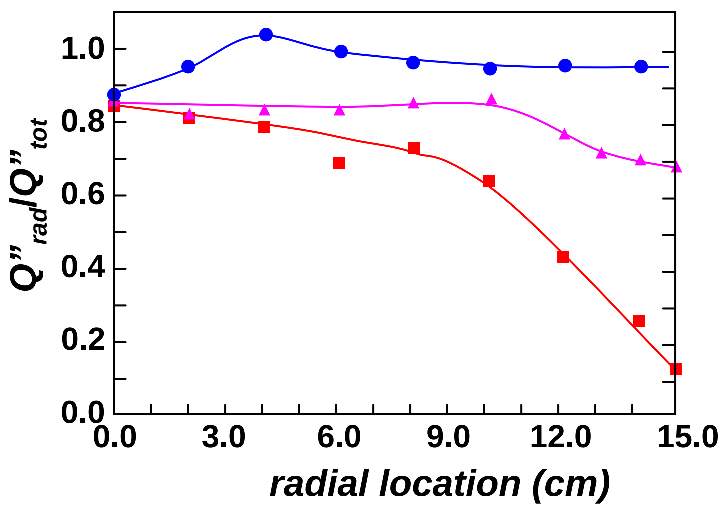
- **Program Manager at NIST**
  - Dr. Jiann Yang

Radiation Feedback to Fuel Surface

Images of 45 cm pool fires (from BFRL)



Measurements of radiative feedback in 30 cm liquid pool fires Hamins et al. (1994)



Fraction of heat feedback to pool due to radiation

Toluene	$Q_{rad}/Q_{tot} = 0.96$
Heptane	$Q_{rad}/Q_{tot} = 0.80$
Methanol	$Q_{rad}/Q_{tot} = 0.55$

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Objectives of the Program

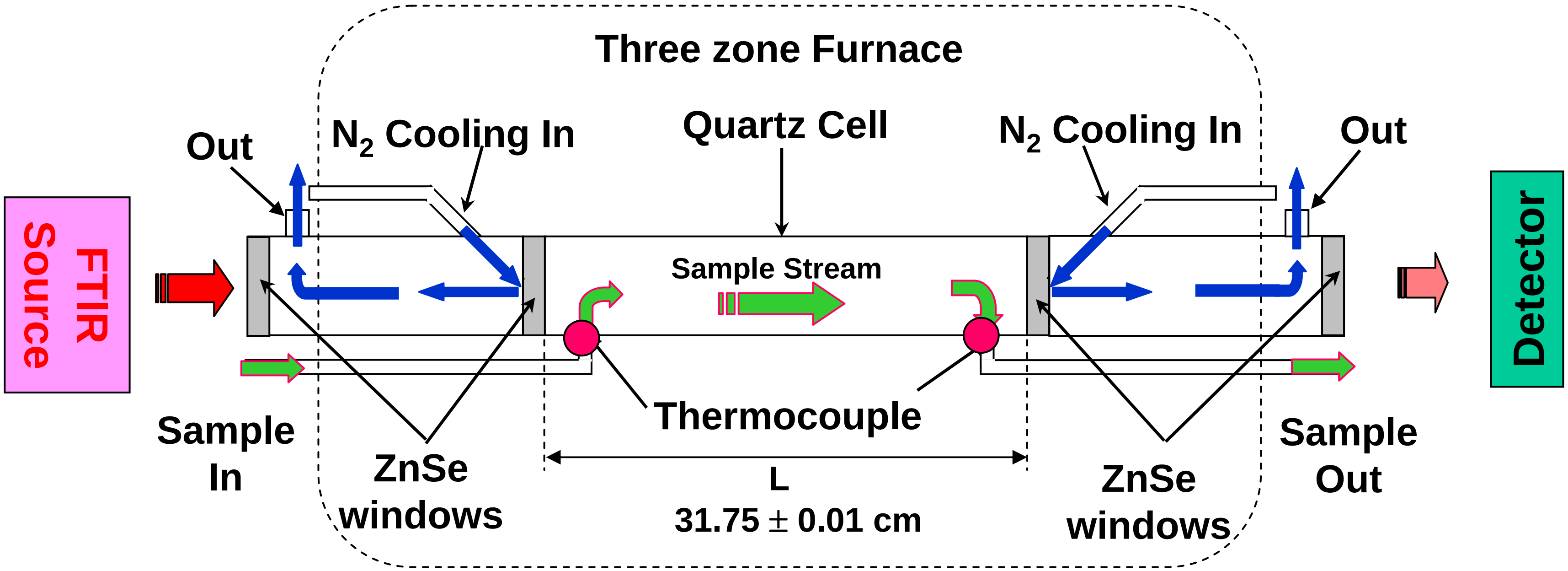
- Develop methodology for building absorption coefficient (κ) database for species in fuel rich cores of fires
- Evaluate the impact of fuel absorption on radiative transport in pool and other large-scale fires
- Integrate the database into Fire Dynamic Simulator for more effective radiative transport calculations
- Demonstrate the effectiveness of radiation database for extracting species profiles in fires

Absorption Coefficient Database

- **New database from current study expands RADCAL**
  - *Improved resolution as well as increased number of species*
- **Implements user-defined spectrally resolved tables with fits for finding absorption coefficients at any arbitrary temperature**

	HITEMP	RADCAL	New Database
Study	Rothman et al. (2003)	Grosshandler (1993)	This study
Temperature	$\leq$ 1000 K	$\leq$ 2000 K	$\leq$ 1000 K with possible extrapolation
Species	3	5	12+
Combustion products	CO_2, H_2O, CO	CO_2, H_2O, CO, Soot	CO_2, H_2O, CO
Fuel	N/A	CH_4	CH_4, CH_3OH, C_2H_4, C_2H_6, C_3H_6, n-C_3H_8, $C_5H_8O_2$, n-C_7H_8, n-C_7H_{16}

High Temperature FTIR Absorption Measurements



- **Gaseous Species – n-C_3H_8, C_3H_6, C_2H_6 , C_2H_4, CH_4**
- **Liquid Fuels – n-C_7H_{16}, CH_3OH, C_7H_8, $C_5H_8O_2$**
- **Absorption measurements from 300 to 1000 K for 3 concentrations.**

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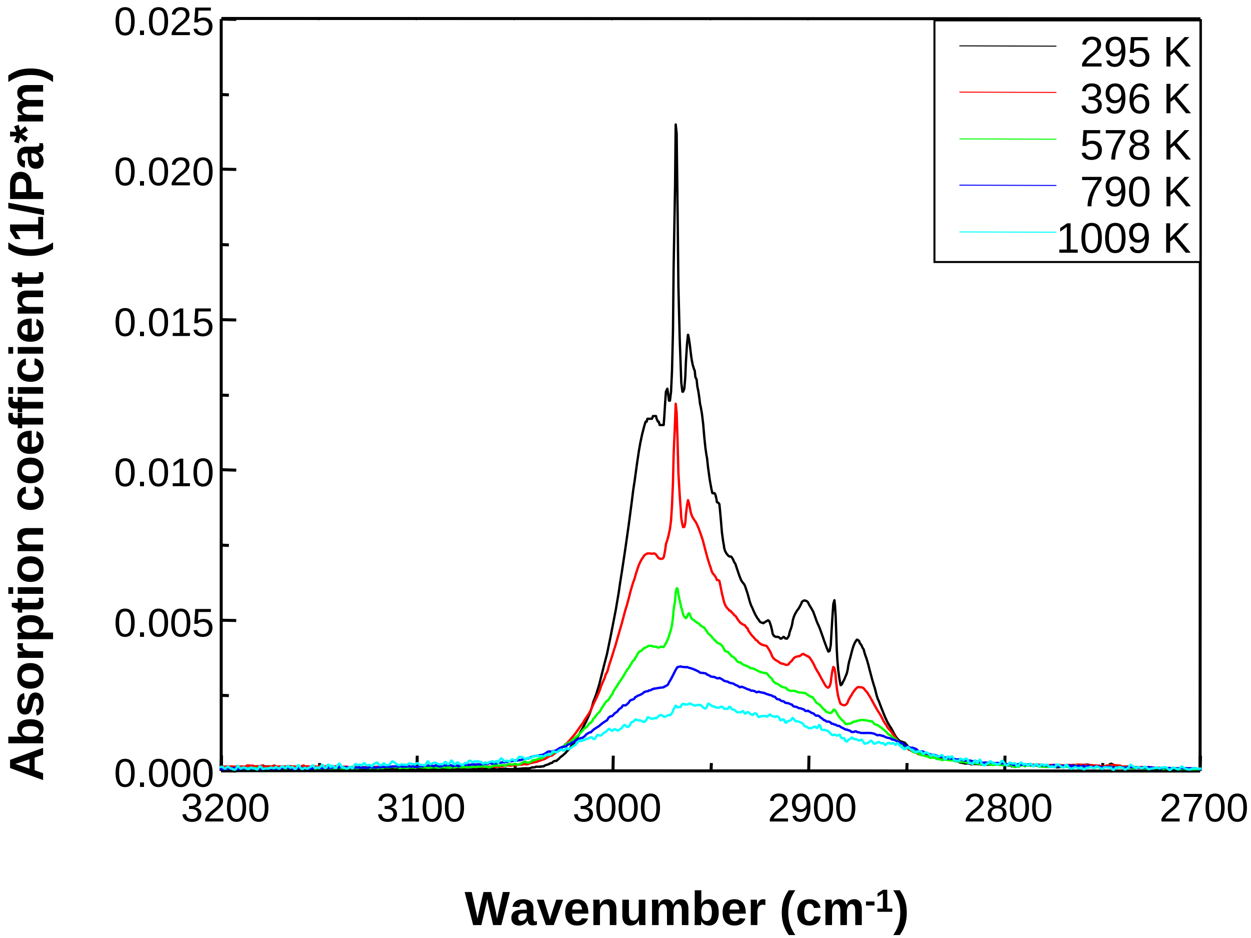
Absorption Measurements for Propane

Measured temperature-dependent spectral absorption coefficient for C_3H_8 in C-H stretching region



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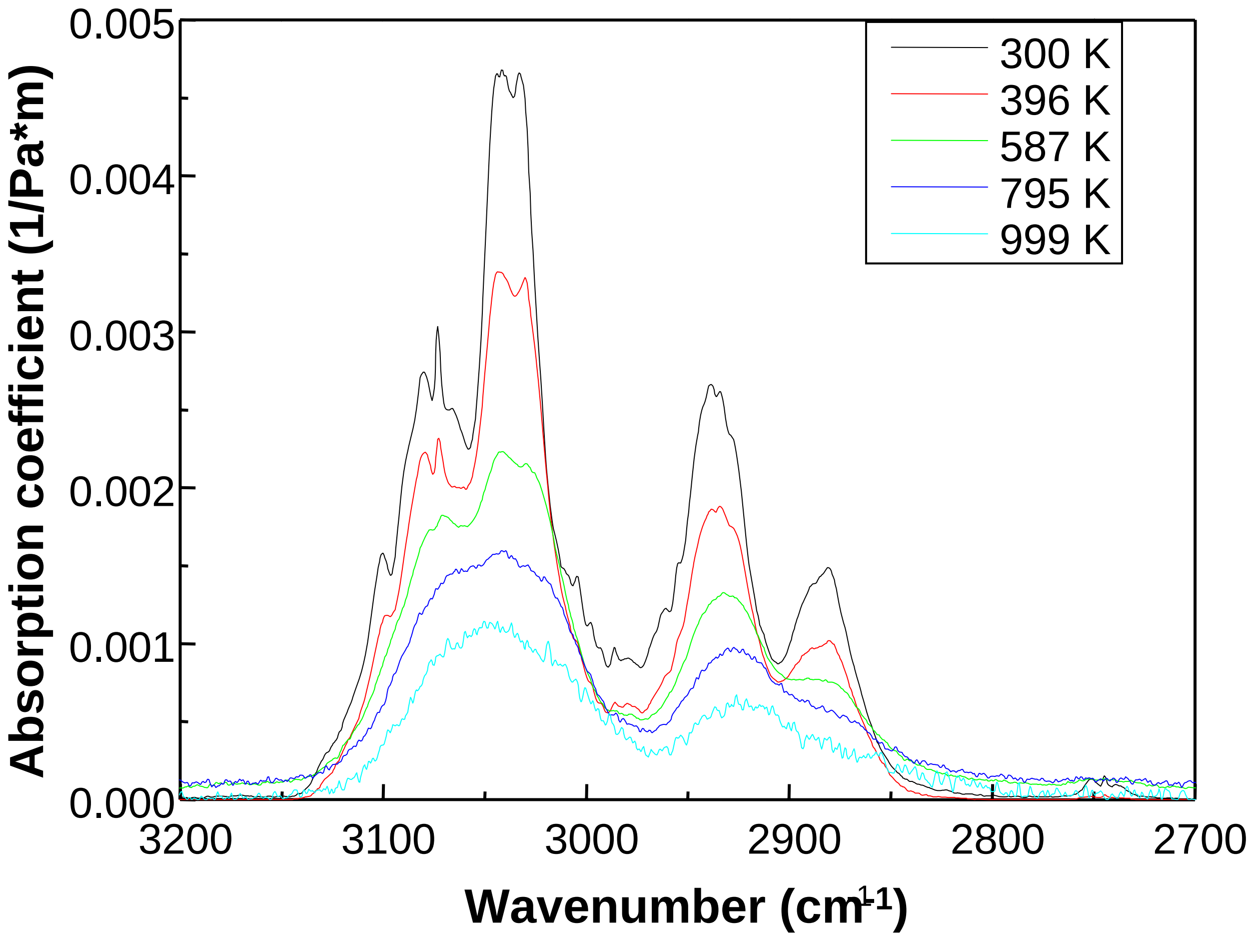
Absorption Measurements for Toluene

Measured temperature-dependent spectral absorption coefficient of C_7H_8; CH_3- and =CH stretching bands



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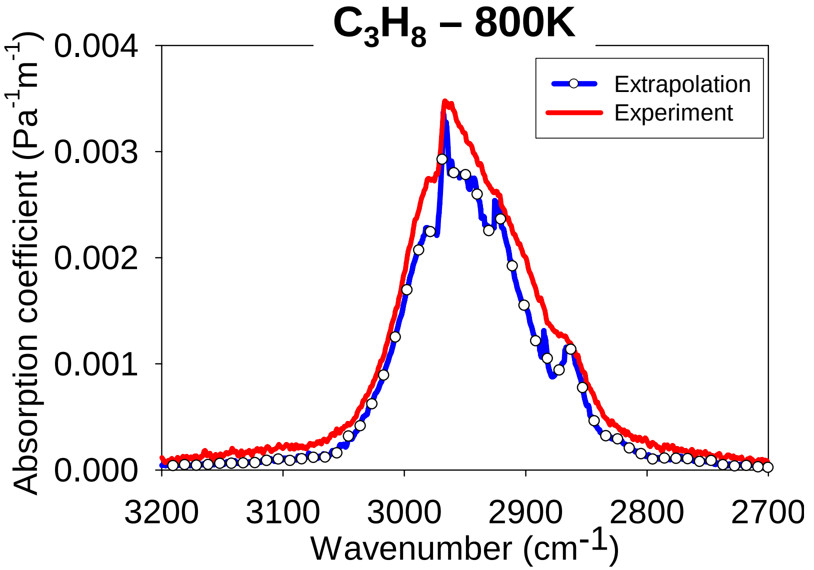
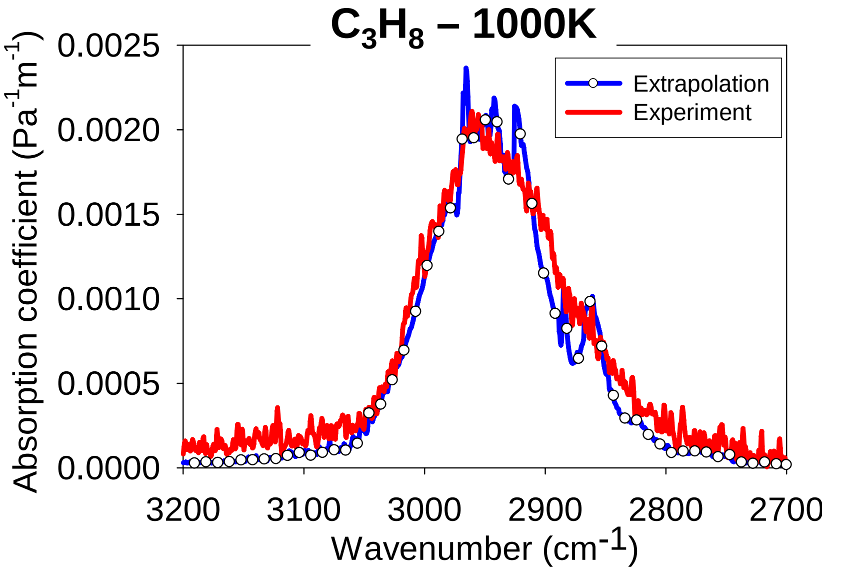
Fitting Procedure for Temperature-Dependent Absorption Coefficient Calculations

- **Temperature fit developed by assuming semi-empirical expression (developed by Fuss et al. 2001) with three fit parameters S_0, ν_r, and *n***
  - Fails to capture high-temperature band-broadening

$$\kappa_\upsilon = \frac{S_0 \cdot \nu \cdot \left[1 - \exp\left(-\frac{1.439 \cdot \nu}{T}\right)\right] \cdot \exp\left(-\frac{1.439 \cdot \nu_r}{T}\right)}{T^n}$$





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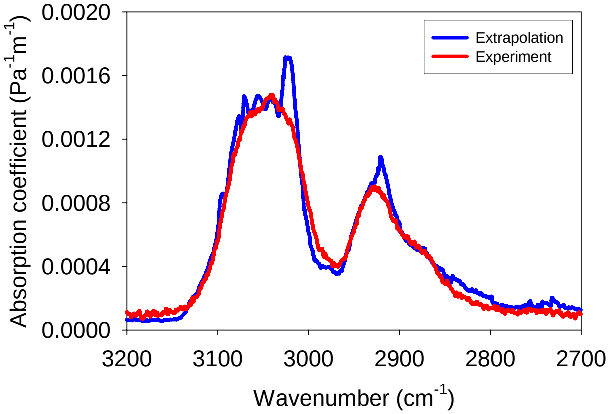
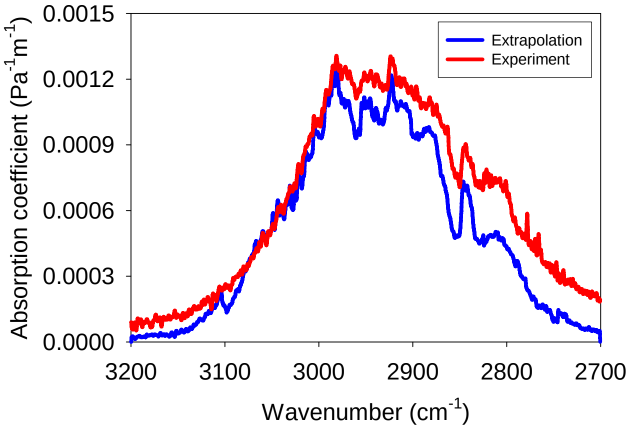
Comparing High Temperature Measurements with Fittings

Comparison of C_7H_8, CH_3OH, and n-C_7H_{16} data at 800 K with 1 cm^{-1} resolution to fits extrapolation from 300-600 K measurements

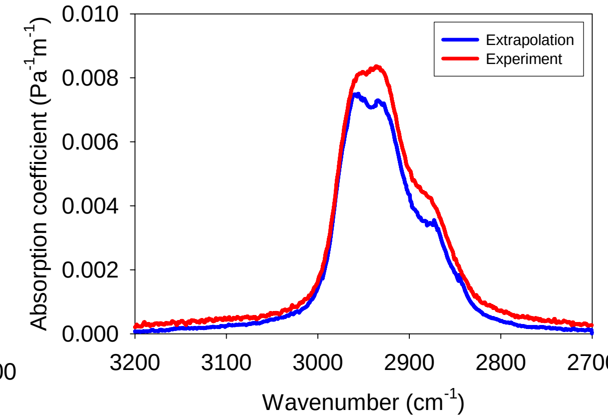
Toluene



Methanol



Heptane



Errors of the integrated absorption coefficients at 1 cm^{-1} resolution

Toluene: + 5.3% ***Methanol: - 20.1%*** ***Heptane: - 17.4%***

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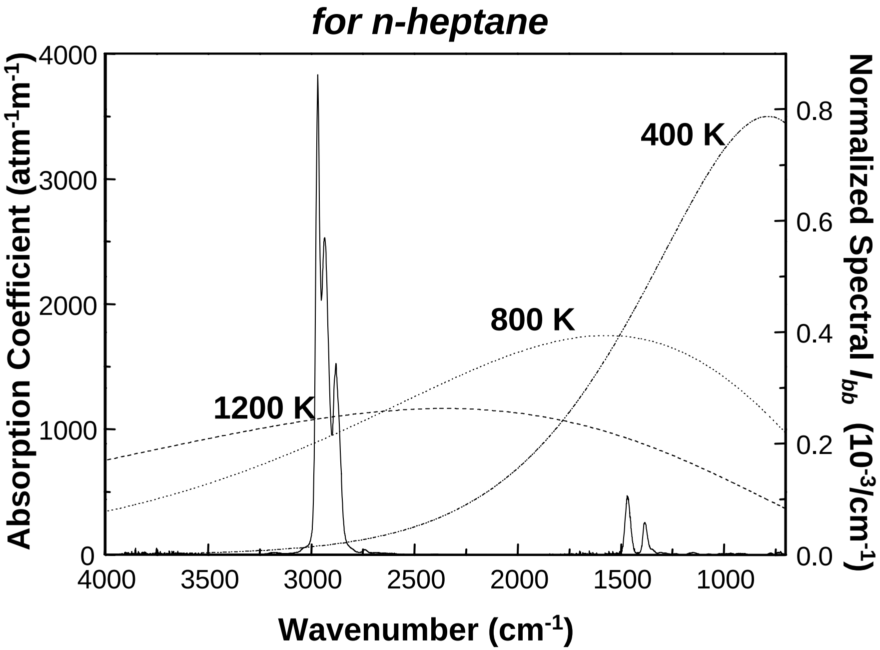
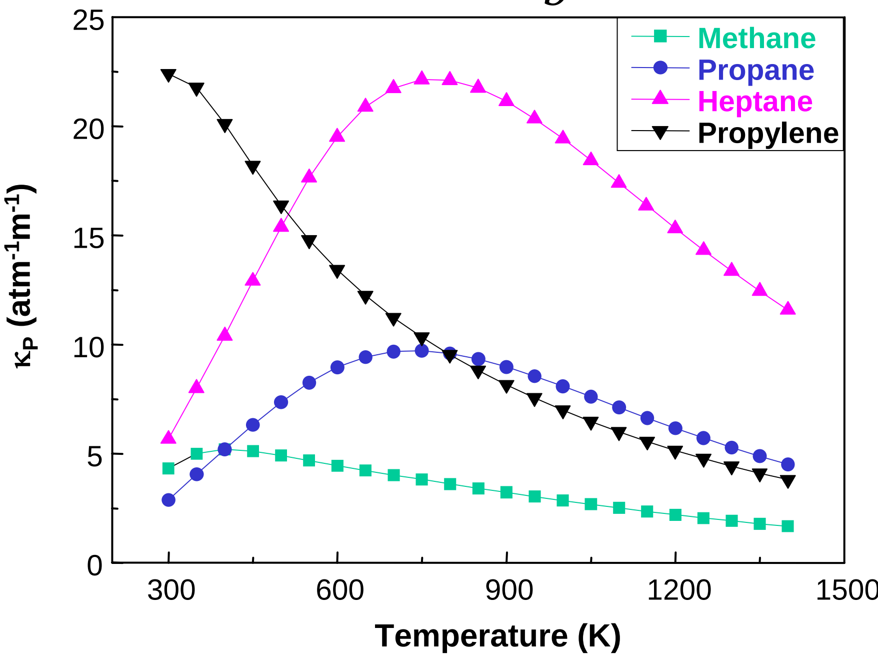
Integrated Planck Mean Absorption Coefficient

- **Due to coincidence of absorption bands with peaks in blackbody radiation at different wavenumbers non-monotonic behavior of Planck mean absorption coefficient is observed.**

$$\kappa_p = \frac{\int_0^\infty \kappa_\lambda I_{b\lambda} d\lambda}{\sigma T_b{}^4}$$





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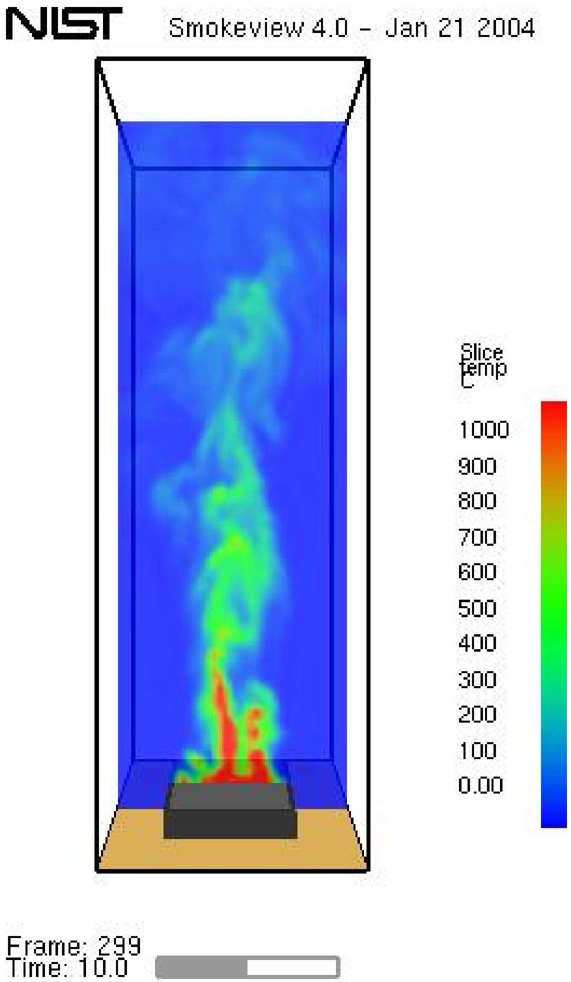
Use of FDS for Incident Thermal Radiation Feedback Analysis

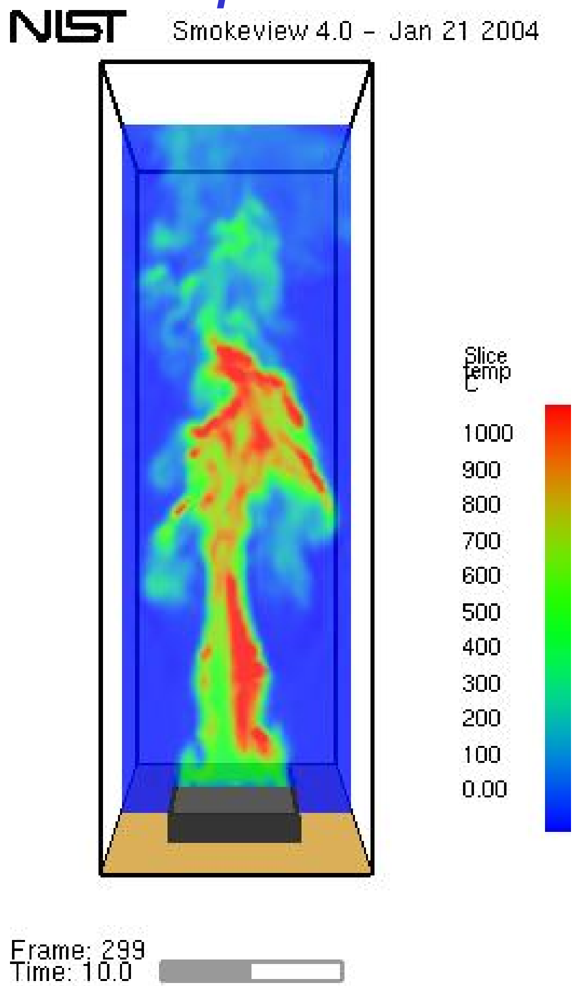
- **Use Fire Dynamic Simulator (FDS 4.02) to generate species and temperature profiles in 30 cm diameter pool fires**
  - profiles determined with 10 s of averaging in computational time after steady-state achieved in LES simulations
  - three fuels studied (CH_3OH as shown here, C_7H_{16}, C_7H_8)
- **Send FDS centerline results to Matlab-based code for doing 1-D centerline radiative transport calculations**
  - Use fuel specific temperature-dependent and independent absorption coefficients for spectrally-resolved radiation calculations
    - *FDS incorrectly assumes all fuels have CH_4 like absorption*
  - Use different flame boundary conditions for calculations
    - *Emission from species concentrations calculated by FDS at selected flame temperature –* $I_{species}$
    - *Plus blackbody emission at 1400 K for fuels with high degrees of sooting (heptane and toluene) –* I_{BB}

FDS Calculated Temperatures in Pool Fires of Methanol, Heptane, and Toluene

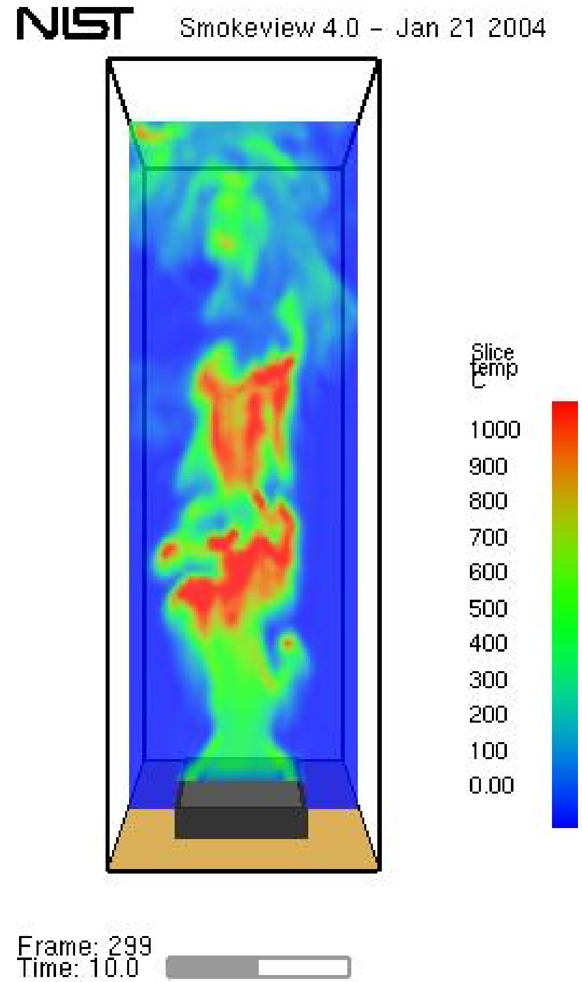
Methanol



Heptane



Toluene



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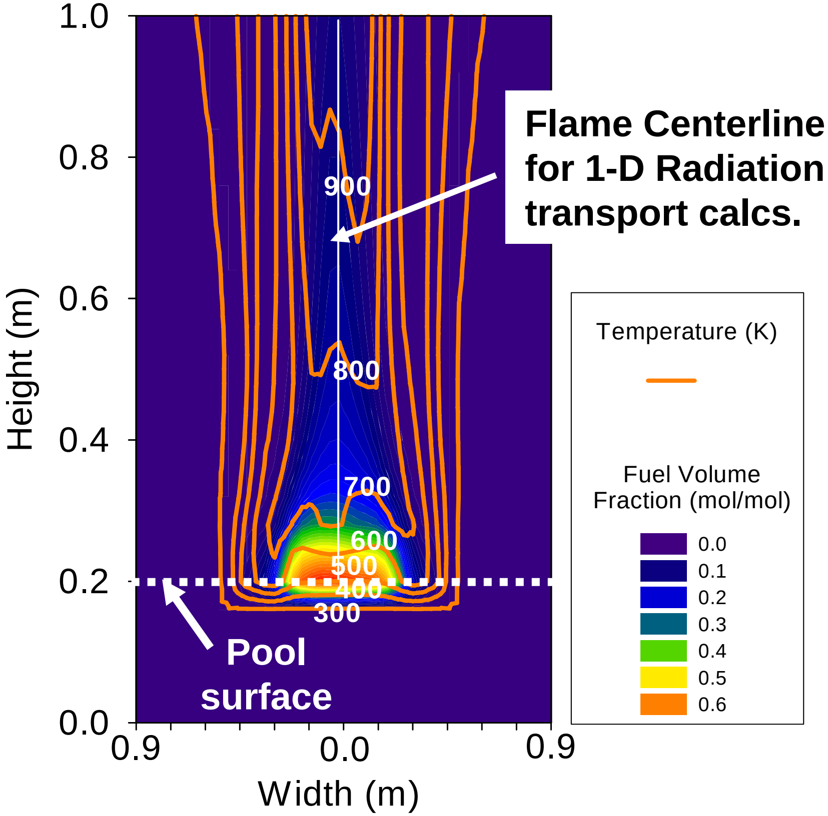
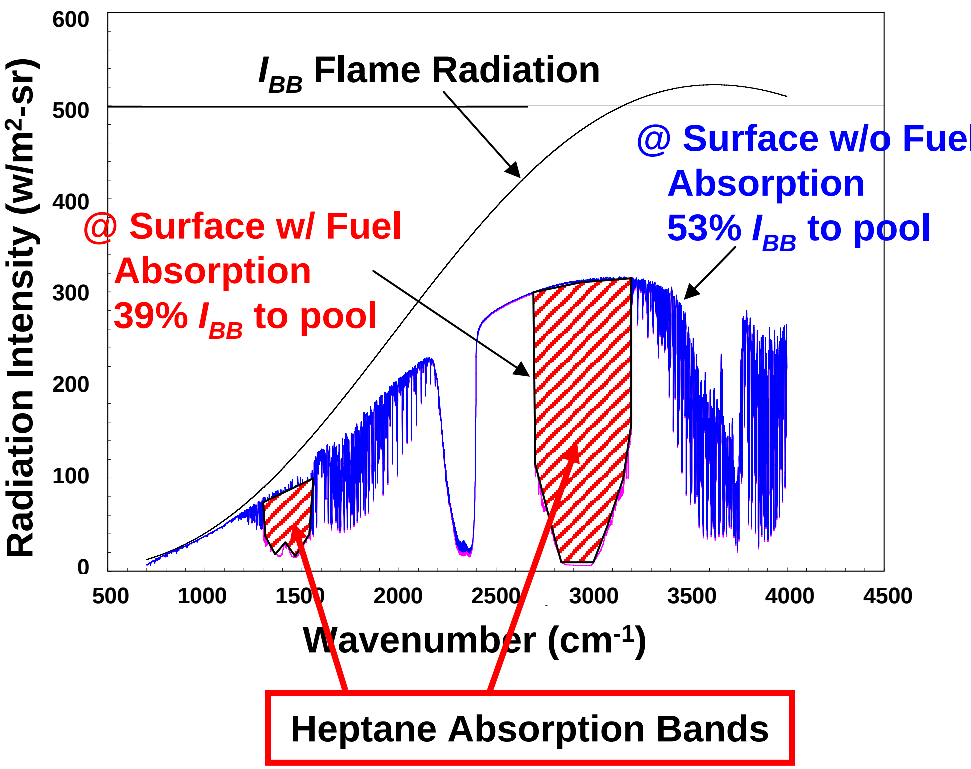
Radiation Feedback to Fuel Surface

Temperature/Fuel contour plot of 1 m heptane pool fire using FDS

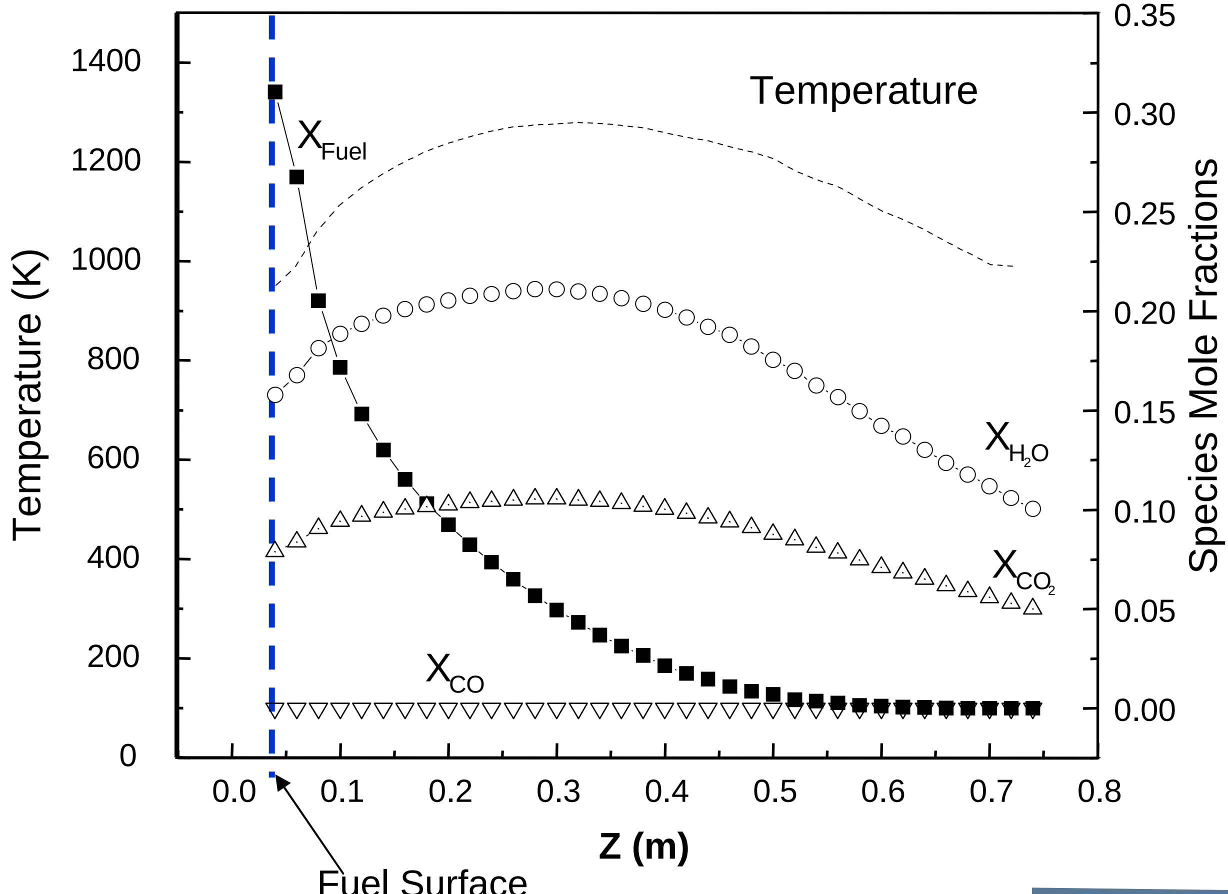


1-D Heptane-Pool-Fire Radiation Transport Calculations Along Flame Centerline



Methanol Pool Fire Simulation Results

Time-averaged temperature and mole fraction of fuel and products as a function of height for 0.3 m methanol pool fire.

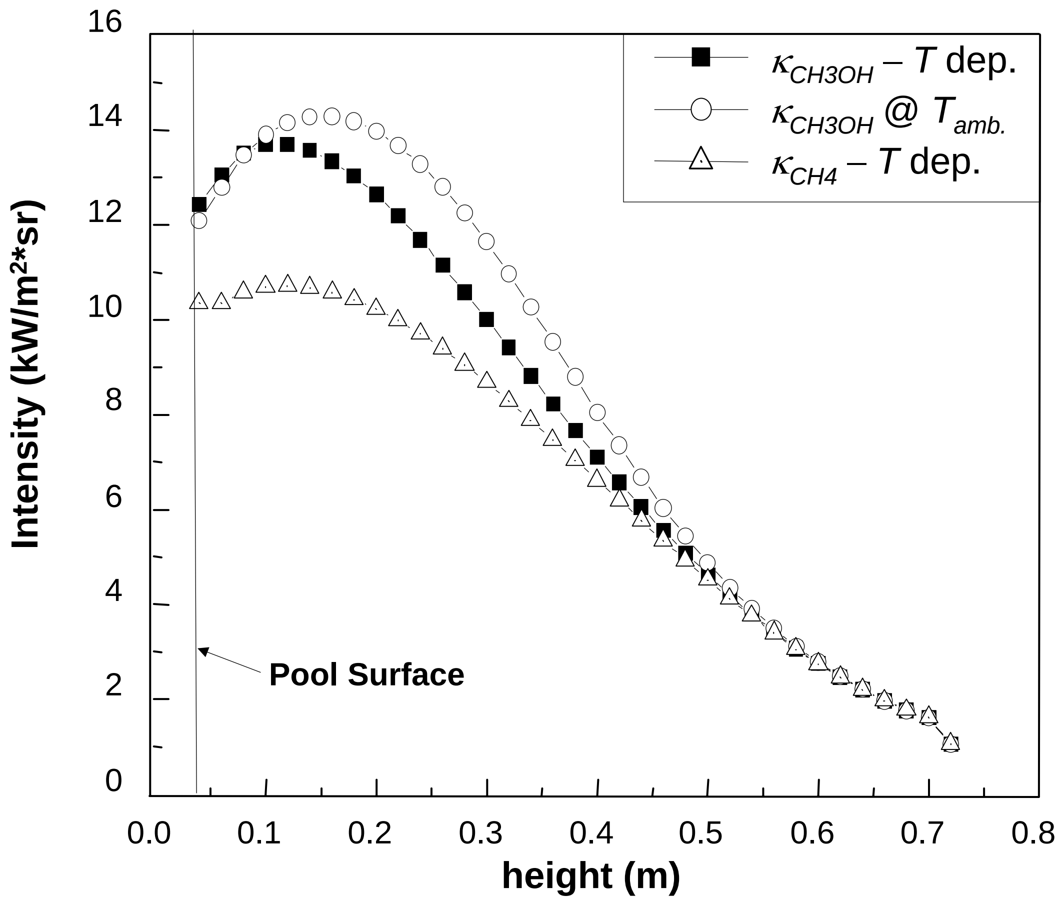


Radiation Calculations for Methanol Pool Fire

- **Integrated directional radiation intensity vs. height for different models of fuel absorption coefficient for 0.3 m methanol pool fire.**

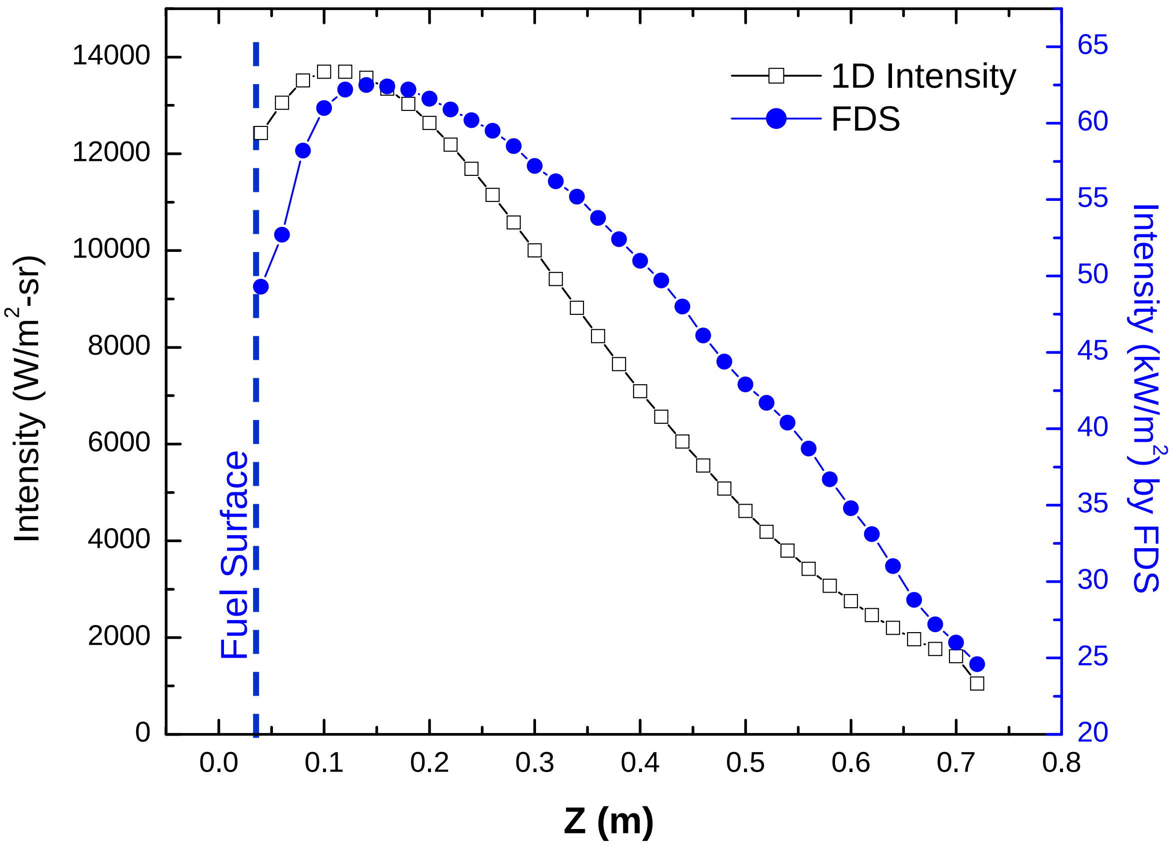
- **Temperature-dependent κ_{CH3OH} gives outstanding agreement with experiments by Klassen et al. (1996)**
  - ***12.2 kW/m^2*sr for calcs.***
  - ***12.4 kW/m^2*sr for expts.***

- **Poor agreement between calculations and experiments with sooty pool fires of heptane and toluene**



Radiation Calculations for Methanol Pool Fire

- **Comparison of radiation intensity of 0.3 m methanol pool fire calculated by 1-D transport equation and FDS which uses $\kappa_{methane}$.**



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Summary and Conclusions

- **Established high temperature FTIR experimental set-up and procedure and measured various fuel absorption coefficients for temperatures up to 1000 K.**

- **Developed calculation technique to interpolate and for some cases extrapolate absorption coefficient (κ) at high temperatures.**

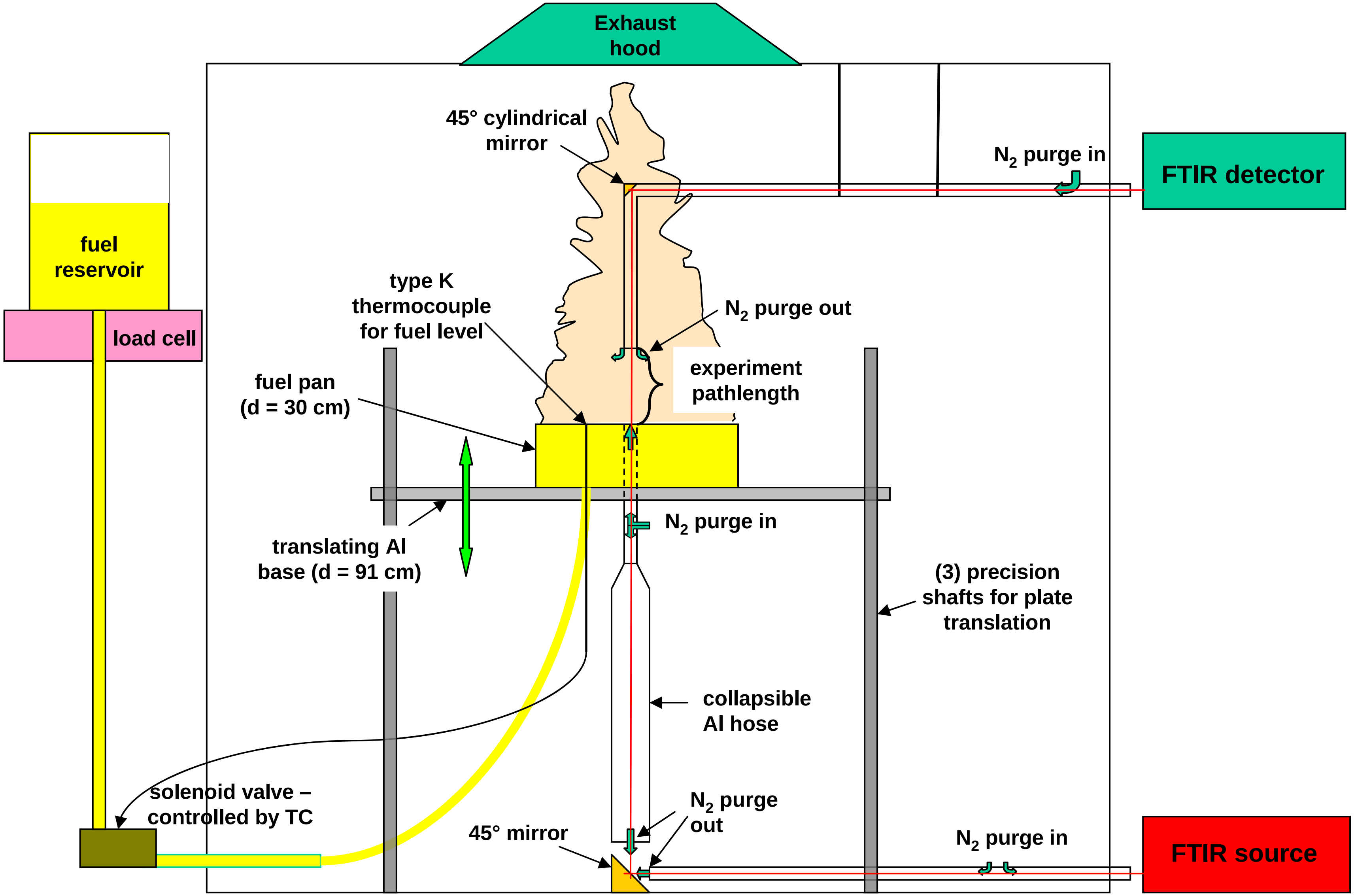
- **Developed new κ database for fuels and combustion products.**
  - Analyzed the Planck mean absorption coefficient.

- **Evaluated radiation intensity at fuel surface with the database solving 1 D radiative transport equation (RTE) at flame centerline.**
  - Used FDS as a tool to generate specie and temperature distribution.
  - Solved the RTE to analyze radiation intensity at fuel surface for methanol, heptane, and toluene 0.3 m pool fire.
  - Soot models and temperature calculations must be improved to better predict radationa intensity for heptane and toluene.
  - Fuel dependency of absorption coefficient more important for small pool calculations than temperature dependency.

Proposed Further Work

- **Investigate radiation transport at gas and liquid interface.**
- **Incorporate new measurements with fitting parameters into user-expandable RADCAL-like database**
- **Complete measurements of well-defined surrogates for common liquid fuels such as gasoline**
- **Program the database and user expandibility into Fire Dynamics Simulator and explore how new radiation information affects incident heat flux on fuel surface and mass burning rates.**
- **Take measurements *in situ* of IR transport through liquid pool fires along pool fire centerline.**
  - Attempt species reconstruction based on spectrally resolved radiation transport measurements for incident radiation flux.

Pool Fire Radiation Measurements with *in situ* FTIR



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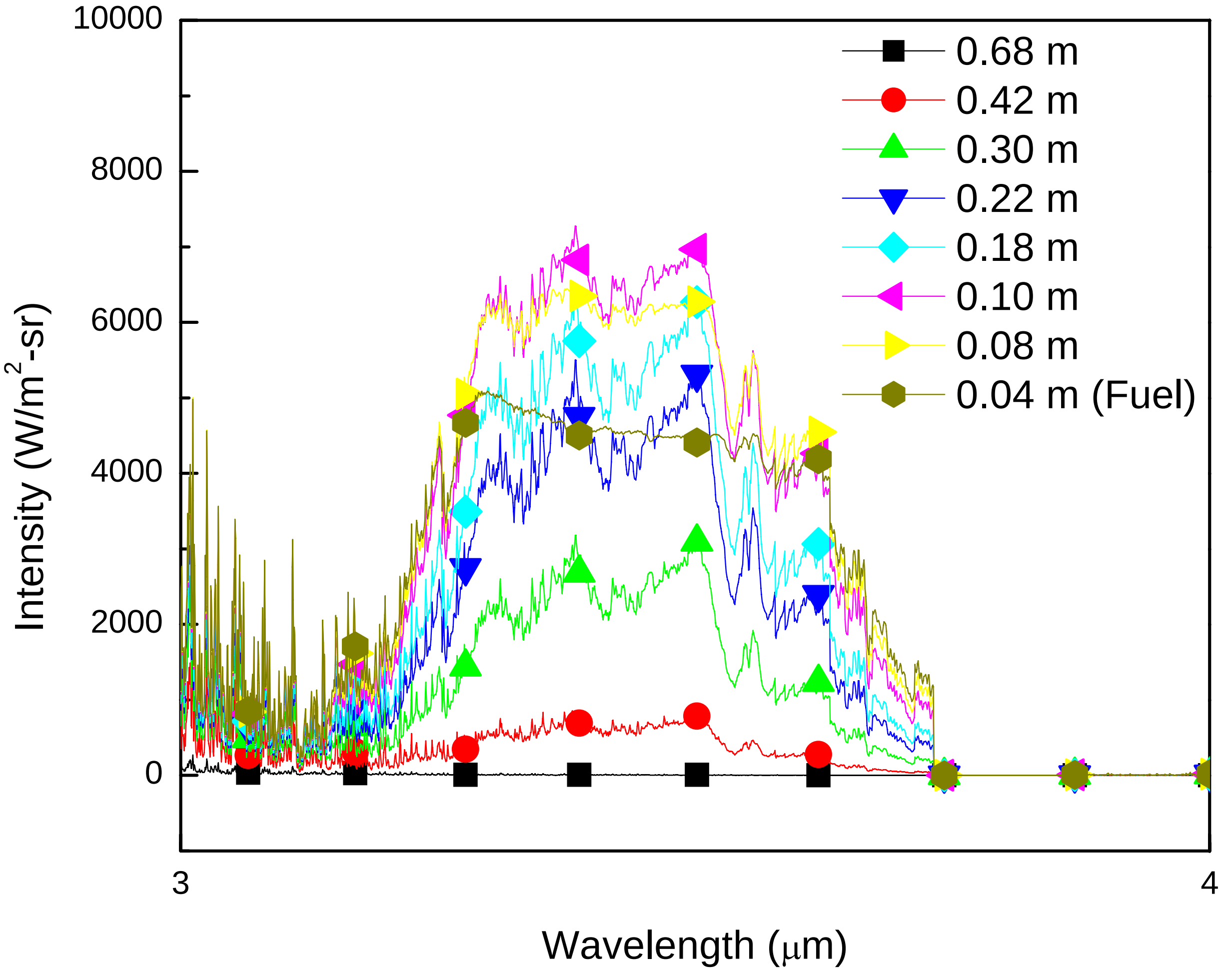
Challenge in Reconstructing Fuel Composition as a Function of Height with *in situ* FTIR Measurements

Spectral radiation intensity of C-H stretching of methanol about 3.4 mm (3000 cm^{-1}) as a function of height



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Previous Temperature Dependent Radiation Absorption Measurements

- **Tien and coworkers (1970's and 80's)**
  - acetylene (C_2H_2), methane (CH_4), propylene (C_3H_6),
  - methyl methacrylate (MMA, $C_5H_8O_2$)

- **Fuss et al. (1996, 1999)**
  - methane (CH_4), ethane (C_2H_6), n-propane (C_3H_8), n-butane (C_4H_{10})